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GC/MS (Gas Chromatograph/Mass Spectrometer) Data Management Process Part 1. User's Guide, Version 1.0

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A GC/MS DATA MANAGEMENT PROCESS

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Part I

User's Guide
Version 1.0

by

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16. ABSTRACT

The GC/MS Data Management Process (DMP) is an example process for reducing measurement and identification data produced by a GC/MS to that necessary for input to the EPA sample file control system. This example is structured for a Finnigan Incos Data System.

The user's guide (Part I) explains the commands available to the user and the resulting outputs. It explains the links between the modules. Examples are also provided for assistance. Some modules which were intended to be part of this package are not yet available in Version 1.0.

A companion report (Part II) documents those programs.

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FOREWORD

Environmental measurements are required to determine the quality of ambient waters and the character of waste effluents. The Environmental Monitoring and Support Laboratory - Cincinnati, conducts research to:

- Develop and evaluate methods to measure the presence and concentration of physical, chemical, and radiological pollutants in water, wastewater, bottom sediments, and solid waste.

- Investigate methods for the concentration, recovery, and identification of viruses, bacteria and other microbiological organisms in water; and to determine the responses of aquatic organisms to water quality.

- Develop and operate an Agency-wide quality assurance program to assure standardization and quality control of systems for monitoring water and wastewater.

- Develop and operate a computerized system for instrument automation leading to improved data collection, analysis, and quality control.

This user's guide was developed in the Advanced Instrumentation Section of the Environmental Monitoring and Support Laboratory (EMSL), Cincinnati, as an example process for reducing measurement and identification information from a gas chromatograph/mass spectrometer (GC/MS) data system. This data reduction system packages production data for the EPA sample file control system.

Robert L. Booth

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ABSTRACT

This users guide explains the application of the GC/MS data management process. This system is an example of a process for reducing measurement and identification data from a gas chromatography/mass spectrometer data system to the requirements for input to the EPA sample file control system. This example is built to run on a Finnigan Incos Data System.

This guide explains the commands available to the user and the resulting outputs. It explains the links between the modules. Examples are also provided for assistance. Some modules which were intended to be part of this package are not yet available in Version 1.0.

A companion report (Part II - Program Documentation) is also available to further explain the software utilized.

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SECTION 1

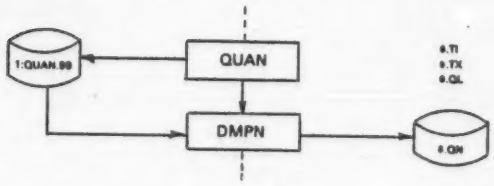
INTRODUCTION

The GC/MS Data Management Process (DMP) is an enhancement to the Finnigan INCOS GC/MS data system. The data acquisition mode of the INCOS data system is called MSDS. The > symbol is the terminal prompt in MSDS. For additional information see the Finnigan INCOS User's Manuals. The primary DMP functions facilitate the gathering and reduction of sample measurement and identification data, the reporting of results and quality control assessments and the packaging and transmission of reduced data to the EPA Sample File Control (SFC) system. A special feature of the DMP system performs replicate statistics computations and reporting on a well specified set of samples. The functions of the DMP system and the associated data and report files are shown in Figure 1.1.

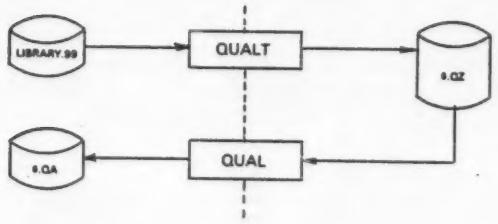
Briefly stated, the DMP system assists the analyst by generating quantitative and qualitative identification reports on a particular sample and combining the information into a reduced data file. All other DMP processes are performed with these reduced data files.

The DMP system uses a sample-naming convention in order to identify the various types of samples being measured in the laboratory. The following codes identify each sample type managed by DMP:

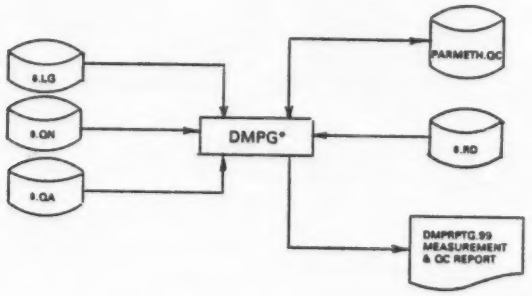
a) Creating QUAN files



b) Creating QUAL files

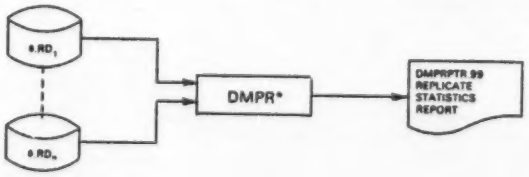


c) Gathering data and generating QC and measurement reports

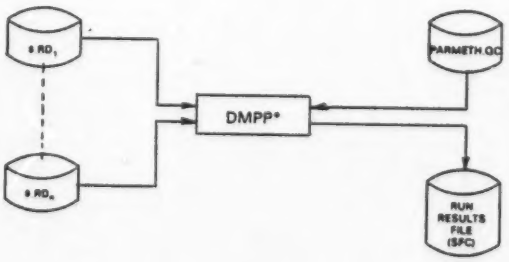


d) Editing QC method template and generating contents

e) Generating replicate statistics report



f) Generating SFC run results files



*NamoList may be used for batch process

Figure 1.1 Primary Data Management Functions

U	unknown sample
D	duplicate of unknown sample
F	spike of unknown sample
C	control standard
R	reagent blank
N	non-SFC sample
S	calibration standard

These types of samples are described in the SFC data element dictionary. The letter codes noted above are used as sample-name terminators. For example, the time-intensity file name for a particular unknown sample might be O:GARBAGEU.TI. The log file for the sample would then be named O:GARBAGEU.LG and the QUAN list and library list for the sample would be similarly identified. In general, the sample name must follow the convention such that its form is

D:SAMPLIDNT .EX

SAMPLIDNT can be up to nine characters long and the position must be filled with a U, D, F, C, R, N or S character. The DMP system presumes that a file name not ending in any of these characters is a non-SFC or N-type sample.

The DMP system acts on each type of sample differently. Unknowns are processed to obtain concentrations. However, since an unknown may be both

duplicated and spiked, the DMP system automatically examines the disk contents for D or F forms of the unknown sample name. If it finds a spike or duplicate of the unknown, it will record the data and also produce spike and/or duplicate quality control reports. The sample identification scheme for the DMP reporting system is shown in Table 1.1. The file extensions shown in the table (that is, .QN, .QA, and .RD) will be described in later sections of this guide.

In order to perform its functions, the DMP system maintains quality control method template files (QC/MT)which are the hub of the DMP system. The QC/MT serves the system by providing quality control and method related data to the system during the processing of sample data files. The QC/MT contains compound names and CAS numbers for a fixed set of analytes measured by a given method. Quality control assessment criteria are linked to a given method and are, therefore, contained in the QC/MT. Finally, the QC/MT contains use codes which identify particular analytes as surrogate spikes or internal standards.

This booklet will describe the use of the DMP system. It contains many figures and demonstration sessions. All underlined segments identify user responses to computer prompts. All responses are terminated with a carriage return by the user. The CONTROL D option is usually available to the analyst at every prompt. The system responds to a CONTROL D by exiting to MSDS unless otherwise noted. Almost all computer prompts have a default response. If the analyst just presses the carriage return in response to a

TABLE 1.1 - SAMPLE/FILE IDENTIFICATION SCHEME FOR THE DMP REPORTING SYSTEM

SAMPLE TYPE	SFC QC CODE	REVERSE SEARCH QUANTIFICATION FILE NAMING	FORWARD SEARCH QUALIFICATION FILE NAMING	REDUCED DATA FILE NAMING
CALIBRATION STANDARD	STD	SAMPLIDNTS. QN	NONE	SAMPLIDNTS. RD +
UNATTACHED OR ORIGINAL UNKNOWN	LD1, LSO LDX OR	SAMPLIDNTU. QN	SAMPLIDNTU.QA	SAMPLIDNTU. RD
LABORATORY DUPLICATE	LD2	SAMPLIDNTD. QN	NONE	*
LABORATORY SPIKE	LSF	SAMPLIDNTF. QN	NONE	*+
LABORATORY CONTROL STANDARD	LCM	SAMPLIDNTC. QN	NONE	SAMPLIDNTC. RD *+
LABORATORY REAGENT BLANK	LRB	SAMPLIDNTR. QN	NONE	SAMPLIDNTR. RD *
NON-SFC SAMPLE	NON #	SAMPLIDNTN. QN	SAMPLIDNTN. QA	SAMPLIDNTN. RD

NOTES:

+ - IMPLIES THAT KNOWN VALUES ARE NEEDED FOR PROPER RECOVERY COMPUTATION.

* - IMPLIES THAT QUALITY CONTROL LIMITS ARE NEEDED FOR APPROPRIATE QC ASSESSMENTS.

- THESE CODES ARE NOT TRUE SFC CODES. STANDARD AND NON-SFC SAMPLE RESULTS WILL NEVER BE SENT TO THE SFC SYSTEM.

prompt, the computer will assume that the analyst is selecting the answer surrounded by square brackets. For example, a prompt ending in the characters '[H]>' may be answered with a carriage return. In this case the program will assume that the analyst needs help and will display more information on the available options.

The DMP system is an interactive command structured system. It cannot be invoked through an MSDS procedure. It must be called directly from MSDS by the analyst. All major functions of the DMP system utilize namelists to facilitate batch processing and reporting.

SECTION 2

GENERATING QUANTITATIVE AND QUALITATIVE IDENTIFICATION FILES FOR DMP PROCESSING

The DMP system uses quantitative and qualitative identification report files. These files are produced by MSDS either directly or through user procedures.

The quantitative file (QUAN .99) is generated with the MSDS QUAN command. The following procedural segment is required to produce DMP compatible quantitation files:

```
.
.
.
> QUAN (...F2...)/K
> DMPN
.
.
.
```

The '/K' instructs the system to produce a disk file called QUAN.99 which contains the report information. The 'F2' option instructs the system to produce a response list segment along with the normal quantitation segment. This option is only required by DMP for the processing of calibration standards and can be omitted for all other sample types. The DMPN command simply copies the QUAN.99 report file to a file named D:SAMPLIDNT .QN. The current sample name ($1) is used as the quantitation file name. Only one

quantitation file can exist for a sample. If a second quantitation is performed on sample data, the old quantitation file is replaced by a new quantitation file.

Qualitative identification files are produced through an interactive SEARCH process. The qualitative identification files are named SAMPLIDNT .QA. Each qualitative identification file should contain names and CAS numbers for compounds found in a sample but not quantified by the method.

SECTION 3

MODIFYING THE SAMPLE LOG FILE

The DMP system requires more than just quantitative and qualitative identification files to process sample data. It also requires volumetric data on the sample measurement as well as sample media and quality control tracking information. The DMP system facilitates the user entry of this information into the sample log file through MSDS procedure DMPL. This procedure should be run immediately after data acquisition (ACQU) has been completed.

An example DMPL session is shown in Figure 3.1. The only mandatory parameters required by the system are the sample source, original sample volume, extract volume, and injection volume. (For calibration standards, only the injection volume is needed.) The units of sample volume will be modified depending on the selected sample source. Analysts not associated with the SFC system may use defaults for the PARMETH (parameter-method) codes. The control standard and reagent blank entries are requested only when the sample is an unknown (U) sample. These entries facilitate quality assurance tracking for groups of unknowns.

The DMPL procedure may be performed on a sample log file more than once. If the file is being modified for a second time, the previously entered parameters will be used as the defaults for the session.

```
LOG FILE MODIFICATION ROUTINE (DMPL)
 SAMPLE NAME [DFTE] > CAL26

 SAMPLE SOURCE CODE:
  1 - WATER
  2 - DRY MATTER (SOIL)
  3 - WET MATTER (SEDIMENT)
  4 - AIR
 OPTION:  [   1] >
 SAMPLE VOLUME: [     1.000] LITERS                >
 EXTRACT VOLUME:[     1.000] MILILITERS            >
 EXTRACTION DATE:   [MM/DD/YY]                     >
 INJECTN VOLUME:    [ 1.000] MICROLITERS           >
 FIXED LIST PARMETH: [      ]                      > PCB8000
 ADDITIONAL COMMENTS
    [                                                          ]
 COMMENT  >

US=      1.000   VE=      1.000   XD= MM/DD/YY   VI=      1.000
PM= PCB8000     CS=               RB=             PV=
CM= COMMENTS
 ACCEPTABLE LOG FILE PARAMETERS [Y]  >  Y
```

Figure 3.1

SECTION 4

THE DATA MANAGEMENT PROCESS COMMAND LEVEL OPTIONS

Almost all DMP functions are accessible by executing the DMPC command at MSDS. DMPC is a master command level which controls user access to the DMP functional modules or programs. The only DMP processes not accessible from DMPC are the DMPN (Section 2) and the DMPL (Section 3) modules. Figure 4.1 shows the options available from DMP command level. The default or HELP option provides a description of each command character. Either the 'X' command or a CONTROL D will cause an exit to MSDS.

The remaining sections of this manual will describe the options available at DMP command level (DMPC).

```
   DATA MANAGEMENT PROCESS COMMAND LEVEL (DMPC)


QC/METHOD TEMPLATE NAME:   [XXXYZMN]   >  PCB80P4
DMP COMMAND (GERPQUXH):  [H]  >  H

DMP MASTER COMMAND SUMMARY:
  G - GATHER SAMPLE DATA AND GENERATE REPORT
  E - EDIT REDUCED DATA FILE
  R - COMPUTE REPLICATE STATISTICS
  P - PACKAGE AND SEND SFC RUN RESULTS
  Q - CREATE AND/OR EDIT QC/MT'
  U - UTILITY OPTIONS
  X - EXIT TO MSDS
  H - HELP PRINTS THIS SUMMARY
DMP COMMAND (GERPQUXH):  [H]  >
```

Figure 4.1 DMPC Menu

SECTION 5

Q - QUALITY CONTROL METHOD TEMPLATE FILE CREATION AND EDITING

The QC/MT file holds compound names, CAS numbers, quality control limits and use codes for all the compound in a fixed quantitation list. The QC/MT file is identified by a generic PARMETH code of seven characters. In order to create or edit a QC/MT file, the user must type a 'Q' at DMP command level.

The DMPQ module will prompt for the analyst's initials and the QC/MT File name. If the file exists on disk, the module will shift control to the edit and report program described in Section 5.2. The following section describes the QC/MT creation process.

5.1 CREATING THE QC/MT FILE WITH DEFAULT PARAMETERS

Creating a QC/MT file is a simple process. An example session is shown in Figure 5.1. The analyst is required to identify a calibration standard quantitation file (that is, *S.QN). The program will certify its existence and count the number of analytes present. All compounds in the list must be quantified so that the internal standards can be identified without ambiguity. The program will alert the analyst if a reference problem is encountered. Once the internal standards have been located, the program prompts for a series of measurement parameters and quality control limits. The prompts preceded by a star (*) require responses that are unit dependent. The analyst is given a final opportunity to approve the preliminary values and then the program creates the QC/MT file with the appropriate number of named compounds and corresponding parameters. The program then shifts control to the edit and report program.

EXAMPLE SESSION
QUALITY CONTROL/METHOD
TEMPLATE CREATION

```
QC/METHOD TEMPLATE EDITOR MODULE (DMPQ)

 YOUR INITIALS:  [INITS] >  DPR  (CR)
 QC/METHOD TEMPLATE NAME  [PCBSET1]   >  PCBSET2 (CR)

YOU ARE CREATING A NEW QC/METHOD TEMPLATE.
PLEASE IDENTIFY A RENAMED QUAN.99 FILE REPRESENTING
A FIXED LIST OF STANDARDS.  ALSO ACCEPT OR MODIFY
THE DEFAULT QC LIMITS FOR THE QC/MT.

QUAN REPORT OR SAMPLE NAME  [ISOMIX05S] >  ISOMIX10S (CR)
QUAN FILE HAS  6 ENTRIES.
  UNITS OF MEASURE:  [UG/L]     > (CR)
* REAGENT MDL:  [     5.00]  > (CR)
* MATRIX MDL:   [     5.00]  > (CR)
* RANGE MINIMUM:          [      5.000]  >  1    (CR)
* RANGE MAXIMUM:          [    500.000]  >  200  (CR)
* DUPLICATE SLOPE:        [      0.100]  >
* DUPLICATE INTRCPT:      [      5.000]  >  2    (CR)
* MEAN REAGENT BLNK:      [  0.00]  > (CR)
* REAGENT STD DEV:        [  2.00]  > (CR)
* SPIKE CONC. ADDED:      [  20.00]  >  10  (CR)
  MEAN SPIKE RECOV:       [ 75.0%] > (CR)
  SPIKE STD DEV:          [ 15.0%]  > (CR)
* CONTROL STD.CONC:       [  20.00]  >  10   (CR)
  MEAN CNT.STD.RECOV:     [  75.0%]  >  (CR)
  CNT.STD.STD.DEV:        [  15.0%]  >  (CR)
 DID YOU MAKE A MISTAKE DEFINING DEFAULTS  N    > (CR)
```

Figure 5.1

5.2 QC/MT EDIT OPTIONS

For all existing QC/MT files, the DMPQ module will provide the user with a mini report on the QC/MT header information. It will then prompt the user for an edit option. The header information and edit options are shown in Figure 5.2a. The three major options facilitate the modifications of the QC/MT (M), the reporting of the QC/MT contents (R), and the update of the QC/MT with limits supplied by the SFC system (S). The 'S' option is described in Section 5.3.

The 'M' or modify command initiates QC/MT file editing. The analyst is first shown the list of subfields which may be edited and is prompted to select a subfield. The program will continue to prompt for subfields until the analyst selects the zero or default response. The program then displays the number of compounds which may be modified and prompts the user for a starting and stopping position for the subsequent edit. Figure 5.2b shows the process of selecting the edit subfields and the edit range. Once the subfield(s) and range have been selected, the program will automatically display the contents of each QC/MT record and then prompt the analyst for the new subfield parameters. Once the analyst has input the values the program will redisplay the record contents and prompt for the analyst's approval. The edit process for one record is shown in Figure 5.2c. The cycle will continue until all records in the selected range have been edited. The CAS numbers must always be entered into the QC/MT via the modification process. The analyst should also be warned against changing the compound name. In order for the DMP system to handle the quantitative report properly, the compound names in the QC/MT field must be identical to those in the quantitation file.

```
                    QC/METHOD TEMPLATE
                        10/27/82


    NAME:  PCB8OP4                          DEFAULT UNITS (U):  UG/L
    DATE CREATED:  09/22/82                 LAST UPDATE:  10/01/82
    CREATED BY:  BGM                        CHANGED BY:  RGM
    NO. OF COMPOUNDS:     21                EDIT SUBFIELDS:  (N)

OPTION (MRSGXH) [H]   > H


QC/MT EDIT OPTIONS:
 M -MODIFY CURRENT QC/MT FIELDS(S)
 R -REPORT CONTENTS OF QC/MT
 S -UPDATE QC/MT WITH SFC SUPPLED LIMITS
 G -GET ANOTHER QC/MT TO PROCESS
 X -EXIT TO DMP COMMAND LEVEL
 D -EXITS TO MSDS

OPTION (MRSGXH) [H]  >
```

Figure 5.2a

```
                    QC/METHOD TEMPLATE
                        09/02/82

    NAME: PCBSET1                              DEFAULT UNITS (U):  UG/L
    DATE CREATED: 09/26/82 LAST UPDATE: 07/30/82
    CREATED BY:  RGM                           CHANGED:  DPR
    NO.OF COMPOUNDS:    6                      EDIT SUBFIELDS:  (N)

OPTION (MRSGXH)  [H]  > M  (CR)

EDIT SUBFIELD INDEX:
 0 -DONE SELECTING SUBFIELDS
 1 -COMPOUND NAME
 2 -CAS NUMBER
 3 -USE CODE
 4 -MDL
 5 -DUPLICATE PARAMETERS
 6 -REGENT BLANK PARAMETERS
 7 -SPIKE PARAMETERS
 8 -CONTROL STANDARD PARAMETERS
TO MODIFY THE PARAMETERS IN A GIVEN
SUBFIELD, JUST ENTER THE SUBFIELD
NUMBER WHEN PROMPTED.  MORE THAN ONE
SUBFIELD MAY BE SELECTED.
 D RETURNS TO EDIT OPTIONS.

SUBFIELD   [0] > 8  (CR)
SUBFIELD   [0] >

THERE ARE   6 COMPOUNDS IN THE QC/MT
PLEASE ENTER THE RANGE YOU WISH TO MODIFY:
STARTING COMPOUND   [  1]  > (CR)
STOPPING COMPOUND   [  6]  > (CR)
```

Figure 5.2b

EXAMPLE EDIT PROCESS

```
COMPOUND NUMBER:    2
(1) 1,1'-BIPHENYL, 2,4,5-TRICHLORO-
(2) CAS  :   15862-07-4          (3) USE CODE:  1=NORMAL SPIKE
(4) METHOD DETECTION LIMITS:     (5) DUPLICATE LIMITS /A/:
    REAGENT MDL:    1.00         MIN (A):      1.000  MAX (B):
    MATRIX MDL:     1.00         SLP (C):      0.100  INT (D):

                                EXPECTED          MEAN       STD.DEV
(6) REAGENT BLANK LIMITS:  /A/                    0.00 U       1.00 U
(7) SPIKED SAMPLE LIMITS:  /A/   10.00 U        100.0 %       10.0 %
(8) CNTRL STANDARD LIMITS: /A/   10.20 U        100.0 %        5.0 %

CONTROL STAND. PARAMS:
 STD.CONC   [   10.20]  > (CR)
 MEAN % RECV [ 100.0% ] > (CR)
 STD.DEV %  [   5.0% ] > 3  (CR)

COMPOUND NUMBER:    2
(1) 1,1'-BIPHENYL, 2,4,5-TRICHLORO-
(2) CAS  :   15862-07-4          (3) USE CODE:  1=NORMAL SPIKE
(4) METHOD DETECTION LIMITS:     (5) DUPLICATE LIMITS /A/:
    REAGENT MDL:    1.00         MIN (A):      1.000  MAX (B):
    MATRIX MDL:     1.00         SLP (C):      0.100  INT (D):

                                EXPECTED          MEAN       STD.DEV
(6) REAGENT BLANK LIMITS:  /A/                    0.00 U       1.00 U
(7) SPIKED SAMPLE LIMITS:  /A/   10.00 U        100.0 %       10.0 %
(8) CNTRL STANDARD LIMITS: /A/   10.20 U        100.0 %        3.0 %

MISTAKES ON DISPLAYED PARAMS [N]  > (CR)
```

Figure 5.2c

A report on the contents of the QC/MT file may be produced with the 'R' command. The report is meant to be stored in a binder. Once an intelligent edit has been performed on the QC/MT field, it becomes a semipermanent part of the laboratory methods material. A portion of a QC/MT file contents report is shown in Figure 5.2d.

If the 'G' option is selected, the program routes control to the start of the DMPQ module and prompts for another QC/MT file name. This allows the analyst to continue editing and reporting on QC/MT files without having to exit to DMP command level.

5.3 UPDATING QC/MT LIMITS WITH SFC SUPPLIED VALUES

The quality control limits contained in the QC/MT file should represent historical patterns. To this extent, it is beneficial to obtain the best values possible for inclusion into the template. A GC/MS laboratory which is linked to the SFC system has the opportunity to supply quality control measurements to the SFC QC data base. By doing so, a historical record may be compiled showing the "real" limits governing quality control assessments. Once a sufficiently large number of points have been fed into the SFC QC data base, the SFC system can provide the DMP system with an updated set of limits. This is done by initiating a process on the SFC computer which dumps the limits for a particular PARMETH code to tape. The tape is formatted so that it can be transferred from tape to disk by the INCOS system. The QC/MT option 'S' can then initiate the assimilation of the limits into the appropriate QC/MT file.

The program to perform this functon has not been implemented.

GC/METHOD TEMPLATE
09/02/82

NAME; PCBSET2
DATE CREATED: 09/02/82
CREATED BY: DPR
NO. OF COMPOUNDS: 6

DEFAULT UNITS (U): UG/L
LAST UPDATE: 09/02/82
CHANGED BY: DPR
EDIT SUBFIELDS: (N)

COMPOUND NUMBER: 1
(1) 1,1'-BIPHENYL, 2,2'-DICHLORO-
(2) CAS : 000000-00-0
(3) USE CODE: 0=NOT SPECIFIED
(4) METHOD DETECTION LIMITS
REAGENT MDL: 5.00
MATRIX MDL: 5.00
(5) DUPLICATE LIMITS /D/:
MIN (A): 1.000 MAX (B): 200.000
SLP (C): 0.100 INT (D): 2.000

	EXPECTED	MEAN	STD.DEV
(6) REAGENT BLANK LIMITS: /D/		0.00 U	2.00 U
(7) SPIKED SAMPLE LIMITS: /D/	10.00 U	75. 0 %	15.0 %
(8) CNTRL STANDARD LIMITS: /D/	10.00 U	75. 0 %	15.0 %

COMPOUND NUMBER: 2
(1) 1,1'-BIPHENYL, 2,4,5-TRICHLORO-
(2) CAS : 000000-00-0
(3) USE CODE: 0=NOT SPECIFIED
(4) METHOD DETECTION LIMITS
REAGENT MDL: 5.00
MATRIX MDL: 5.00
(5) DUPLICATE LIMITS /D/:
MIN (A): 1.000 MAX (B): 200.000
SLP (C): 0.100 INT (D): 2.000

	EXPECTED	MEAN	STD.DEV
(6) REAGENT BLANK LIMITS: /D/		0.00 U	2.00 U
(7) SPIKED SAMPLE LIMITS: /D/	10.00 U	75. 0 %	15.0 %
(8) CNTRL STANDARD LIMITS: /D/	10.00 U	75. 0 %	15.0 %

COMPOUND NUMBER: 3
(1) 1,1'-BIPHENYL, 2,2',5,5'-TETRACHLORO-
(2) CAS : 000000-00-0
(3) USE CODE: 0=NOT SPECIFIED
(4) METHOD DETECTION LIMITS
REAGENT MDL: 5.00
MATRIX MDL: 5.00
(5) DUPLICATE LIMITS /D/:
MIN (A): 1.000 MAX (B): 200.000
SLP (C): 0.100 INT (D): 2.000

	EXPECTED	MEAN	STD.DEV
(6) REAGENT BLANK LIMITS: /D/		0.00 U	2.00 U
(7) SPIKED SAMPLE LIMITS: /D/	10.00 U	75. 0 %	15.0 %
(8) CNTRL STANDARD LIMITS: /D/	10.00 U	75. 0 %	15.0 %

COMPOUND NUMBER: 4
(1) 1,1'-BIPHENYL, 4,4'-DIBROMO-
(2) CAS : 000000-00-0
(3) USE CODE: 3=INTERNAL STND.
(4) METHOD DETECTION LIMITS
REAGENT MDL: 5.00
MATRIX MDL: 5.00
(5) DUPLICATE LIMITS /D/:
MIN (A): 1.000 MAX (B): 200.000
SLP (C): 0.100 INT (D): 2.000

	EXPECTED	MEAN	STD.DEV
(6) REAGENT BLANK LIMITS: /D/		0.00 U	2.00 U
(7) SPIKED SAMPLE LIMITS: /D/	10.00 U	75. 0 %	15.0 %
(8) CNTRL STANDARD LIMITS: /D/	10.00 U	75. 0 %	15.0 %

Figure 5.2d

SECTION 6

G - GATHERING SAMPLE DATA AND GENERATING REPORTS

A major function of the DMP system is gathering sample data and generating reports. In order to initiate this function, the analyst must type a 'G' at DMP command level.

The DMPG module first prompts the user for a QC/MT file name. Any sample processed during the session must coincide directly with the selected QC/MT file. This means that the number, name, and sequence of compounds in the sample quantitation file must be identical to those in the QC/MT file.

The program then prompts the user to identify the entry mode. Two modes are available: one allows individual sample filenames to be entered (M), and the other facilitates name entry by name list (L). Depending on the entry mode, the analyst is required to enter either a sample name or a namelist name. Figure 6.1a shows a demonstration session for the 'G' command.

For each sample, the DMPG module opens and reads the sample log file ($.LG) and the sample quantitation file ($.QN). All compound names in the quantitation file are checked against their counterparts in the QC/MT file. The log file is checked to make sure the user has included the volumetric and quality assurance parameters (Section 3). If the sample is an unknown, the module will also search for accompanying duplicate and spiked sample data. If the sample is an unknown or non-SFC sample, the DMPG module will search for a qualitative identification file ($.QA).

EXAMPLE SESSION DATA GATHERING
AND REPORTING ROUTINE

DATA MANAGEMENT PROGRAM CONTROL ROUTING (DMPC)

```
DMP COMMAND (GERPQUXH): [H]   >

DMP MASTER COMMAND SUMMARY:
  G - GATHER SAMPLE DATA AND GENERATE REPORT
  E - EDIT REDUCED DATA FILE
  R - COMPUTE REPLICATE STATISTICS
  P - PACKAGE AND SEND SFC RUN RESULTS
  Q - CREATE AND/OR EDIT QC/MT
  U - UTILITY OPTIONS
  X - EXIT TO MSDS
  H - HELP PRINTS THIS SUMMARY
DMP COMMAND (GERPQUXH): [H]  > G (CR)

DATE REDUCTION MODULE (DMPG1)

QC/METHOD TEMPLATE NAME [PCB8OP4]  >
NAME LIST (L) OR MANUAL NAME (M) ENTRY [M]  > L  (CR)
NAME OF LIST FILE  PCB8SFSTD   >
NOW PROCESSING PRIMARY SAMPLE: PCB8SF01S
NOW PROCESSING PRIMARY SAMPLE: PCB8SF1S
NOW PROCESSING PRIMARY SAMPLE: PCB8SF5S
NOW PROCESSING PRIMARY SAMPLE: PCB8SF10AS
NOW PROCESSING PRIMARY SAMPLE: PCB8SF20AS
NOW PROCESSING PRIMARY SAMPLE: PCB8SF50S
NOW PROCESSING PRIMARY SAMPLE: PCB8SF100S
NOW PROCESSING PRIMARY SAMPLE: PCB8SF05CS

REPORT GENERATION MODULE (DMPG2)

NOW REPORTING ON PRIMARY SAMPLE: PCB8SF01S
NOW REPORTING ON PRIMARY SAMPLE: PCB8SF1S
NOW REPORTING ON PRIMARY SAMPLE: PCB8SF5S
NOW REPORTING ON PRIMARY SAMPLE: PCB8SF10AS
NOW REPORTING ON PRIMARY SAMPLE: PCB8SF20AS
NOW REPORTING ON PRIMARY SAMPLE: PCB8SF50AS
NOW REPORTING ON PRIMARY SAMPLE: PCB8SF100S
IDOS ERR 57 OP 34 AT 26362 FROM 75
TYPE <CTL-D> TO CONTINUE PROCESSING
 D
NOW REPORTING ON PRIMARY SAMPLE: PCB8SF05CS
```

Figure 6.1a

The data on any given sample is then compressed into a reduced data file ($.RD). Table 1.1 shows the activities of the DMPG module for the various sample types. The data validation and compression process is lengthy so the module displays its status at relatively short intervals. It is suggested that a namelist always be used with this module and that sufficient time be allocated for the process.

Once the DMPG module completes processing a sample or group of samples it transfers control to the report generator. This module reads reduced data files and their corresponding QC/MT files and generates measurement and quality assurance reports on the sample(s). Figures 6.1b through 6.1f show example reports generated for an unknown (U), a duplicate unknown (D), a spiked unknown (S), a reagent blank (R), and a control standard (C). Note that duplicate and spike reports are intimately associated with the parent unknown since all data resides in the unknown's reduced data file.

Once the report module is finished generating reports, it passes control back to the DMP command level (DMPC).

SECTION 7

E - EDITING THE REDUCED DATA FILE

The analyst should have the opportunity to modify any data in a reduced data file. The primary purpose of the edit function, however, is to facilitate the entry of concentration data for compounds which were previously identified as being present in the sample but were not quantified by the method. The QUAL process produces qualitative identification data on an unknown (U) or non-SFC sample (N). This data is included in the reduced data file along with the quantitative data obtained on the sample through the QUAN process. If the analyst elects to "back-quantify" a previously identified compound, or calibrate for compounds found in a sample but not in the original reverse search library, the edit module will allow for the inclusion of this result in the reduced data file.

The edit module has not been implemented.

SECTION 8

R - USING THE REPLICATE STATISTICS MODULE

A major feature of the DMP system is replicate statistics computation and reporting. The replicate statistics module (DMPR) can be accessed by the analyst through the 'R' command at DMP command level. The analyst will be required to identify the item of interest and the names of the reduced data files to be examined. The DMPR module will then produce the report.

Under certain circumstances, the generated statistics can be used to update parameters in the QC/MT file. This process will be described in Section 8.2.

8.1 COMPUTING AND REPORTING REPLICATE STATISTICS

The replicate statistics module (DMPR) first prompts for a QC/MT file name and then prompts for the item of interest or the parameter on which statistics are to be completed. Figure 8.1a shows an example replicate statistics definition session. Each option usually requires a special sample type in order to perform the computations. The next step requires the analyst to identify the reduced data files which will be used to compute the statistics. There are three ways to enter file names into the replicate list. The analyst may type individual reduced data file names into the list or use a namelist to enter a group of names into the list. The third option allows for a "wild card" name to be used to generate file names into the replicate list. To use this last option, the analyst must type a name with a pound sign (#) in it. The DMPR module will replace the '#' with digits from 0 to 9 and include each name in the replicate list. The DMPR module

EXAMPLE REPLICATE STATISTIC
DEFINITION SESSION

```
                DATA MANAGEMENT PROGRAM CONTROL ROUTING (DMPC)

 QC/METHOD TEMPLATE NAME:  [XXXYZMN]   > PCBSET1 (CR)
 DMP COMMAND (GERPQUXH):   [H]   > R (CR)

REPLICATE ANALYSIS MODULE (DMPR1)

 QC/METHOD TEMPLATE NAME  [PCBSET1]   > (CR)
 OPTION (UNCFMTRAH)  [H]   > (CR)

ANALYSIS OPTIONS:
 U -CONCENTRATION FOR UNKNOWNS
 N -CONCENTRATION FOR NON-SFC SAMPLES
 C -CONC.,%RECOVERY,  MDLR FOR CONTROL STANDARDS
 F -RECOVERED CONC.& %RECOVERY FOR SPIKED SAMPLES
 M -CONC.  MDLX FOR MODIFIED MATRIX NON-SFC SAMPLES
 T -REL.RET.TIME FOR ANY NON-BLANK SAMPLE TYPE
 R -RESPONSE FACTOR FOR CALIBRATION STANDARDS
 A -RESPONSE RATIO (AR/CN) FOR CAL.STANDARDS
 OPTION (INCFMTRAH) [H]   > R (CR)
 OPTIONS (KLWH)  [H]   > (CR)

LIST DIFINITION MODES:
 K -KEYBOARD ENTRY OF EACH FILENAME
 L -NAMELIST PLUS KEYBOARD ENTRIES
 W -WILDCARD PLUS KEYBOARD ENTRIES
 OPTIONS (KLWH)  [H]  > L  (CR)
 NAME OF LIST FILE [TAPE]   > ISOMIX (CR)
 DATA FILE NAME  [CR TO EXIT]   > (CR)
 STATISTICAL COMPUTATIONS (DMPR2) (CR)
 PROCESSING FILE: D:  0   1-ISOMIX005S.RD
 PROCESSING FILE: D:  0   1-ISOMIX01S.RD
 PROCESSING FILE: D:  0   1-ISOMIX05S.RD
 PROCESSING FILE: D:  0   1-ISOMIX1S.RD
 PROCESSING FILE: D:  0   1-ISOMIX5S.RD
 PROCESSING FILE: D:  0   1-ISOMIX10S.RD
 PROCESSING FILE: D:  0   1-ISOMIX20S.RD
 PROCESSING FILE: D:  0   1-ISOMIX86S.RD
```

Figure 8.1a

continues to prompt for names until the list has reached a maximum of 25 names or the analyst exits the name entry segment.

Once the names have been specified, the DMPR module verifies each name and either accepts or rejects them. Three or more acceptable names must be found in the list or an error message is displayed and the entire process is restarted. After the names have been verified, the module computes the statistics and generates a report. This process may take a substantial amount of time, depending on the number of replicate files and compounds affected. Example replicate statistics reports for control standards (C) and response factors (R) are shown in Figure 8.1b and 8.1c respectively.

Table 8.1 shows the parameters reported for each type of statistical report.

8.2 UPDATING QC/MT LIMITS WITH COMPUTED STATISTICS

In some cases, the statistics generated by the DMPR module can be used to update limits in the QC/MT file. The program to perform this function has not been implemented.

GC/MS REPLICATE STATISTICS REPORT

ITEM OF INTEREST: CONC.%REC. MDLR QC METHOD TEMPLATE: D:PCBSET1.QC
SAMPLE TYPE: CONTRL ST UNITS OF CONC: UG/L
NUMBER OF REPLICATES: 10 DATE COMPUTED: 07/29/82

SAMPLE IDENTIFIERS USED

ISOMIX10AC ISOMIX10BC ISOMIX10ACC ISMIX10DC ISOMIX10EC
ISOMIX10FC ISOMIX10GC ISOMIX10AHC ISMIX10IC ISOMIX10K

NO.	COMPOUND NAME	CAS NUMBER	AVERAGE VALUE	STANDARD DEVIATION	% REL STDEV	KNOWN VALUE	MEAN %REC	LIMIT RANGE	REAGENT MDL
1	1,1'-BIPHENYL, 2,2'-DICHLORO-	13029-08-8	10.302	0.542	5.3	10.07	102.3	5.4	1.760
2	1,1'-BIPHENYL, 2,4,5-TRICHLORO-	15862-07-4	10.440	0.273	2.6	10.20	102.3	2.7	0.998
3	1,1'-BIPHENYL, 2,2'-,5,5'-TETRACHLORO-	35693-99-3	10.510	0.214	2.0	10.40	101.1	2.1	0.695
5	1,1'-BIPHENYL, 2,2',4,4',5,5'-HEXACHLORO-	35065-27-1	10.551	0.279	2.6	10.14	104.0	2.8	0.908
6	1,1'-BIPHENYL, 2,2',3,4,5,5',6-HEPTACHLORO-	52712-05-7	9.941	0.441	4.4	9.93	100.1	4.4	1.433

Figure 8.1b

RESPONSE FACTOR REPORT

GC/MS REPLICATE STATISTICS REPORT

ITEM OF INTEREST: RESPONSE FACTOR
SAMPLE TYPE: CAL STND
NUMBER OF REPLICATES: 8

QC METHOD TEMPLATE: D:PCBSET1.QC
UNITS OF CONC: UG/L
DATE COMPUTED: 09/01/82

SAMPLE IDENTIFIERS USED

ISOMIX005S ISOMIX01S ISOMIX05S ISOMIX1S MISMIX5S
ISOMIX10S ISOMIX20S ISOMIX86S

NO.	COMPOUND NAME	CAS NUMBER	AVERAGE VALUE	STANDARD DEVIATION	% REL STDEV
1	1,1'-BIPHENYL, 2,2'-DICHLORO-	13029-08-8	11.731	14.459	123.2
2	1,1'-BIPHENYL, 2,3,4-TRICHLORO-	15862-07-4	11.060	13.466	121.7
3	1,1'-BIPHENYL, 2,2',5,5'-TETRACHLORO-	35693-99-3	5.926	7.096	119.7
4	1,1'-BIPHENYL, 4,4'-DIBR I OMO-	92-86-4	1.000	0.000	0.0
5	1,1'-BIPHENYL, 2,2',4,4',5,5'-HEXACHLORO-	35065-27-1	2.778	3.604	129.7
6	1,1'-BIPHENYL, 2,2',3,4 5,5',6-HEPTACHLORO-	52712-05-7	1.308	1.601	122.4

Figure 8.1c

Table 8.1 - Replicate Analysis Categories and Report Parameters

U or N	1.	Concentration for unknowns (U) or non-SFC (N) samples; provides mean, standard deviation, and % RSD on individual analyte concentrations.
C	2.	Concentration, % recoveries and MDLR for laboratory control standards (C); provides mean, standard deviation, and % RSD on individual analyte concentrations and % recoveries; a reagent MDL is also computed.
S	3.	Concentration and % recoveries for laboratory spiked samples (F); provides mean, standard deviation, and % RSD on individual analyte concentrations recovered and % recoveries.
M	4.	MDLX for modified-matrix non-SFC samples (N); provides mean, standard deviation, % RSD and matrix MDL results for individual analyte concentrations; notification is given on questionable MDL's.
T	5.	Relative retention time on any uniform sample type (any); provides mean, standard deviation and % RSD on individual relative retention times.
R	6.	Response factors on calibration standards (S); provides mean, standard deviation and % RSD for individual analyte response factors.
A	7.	Area vs. known-amount ratios for calibration standards (S); provides mean, standard deviation and % RSD for individual analyte area ratios.

SECTION 9

P - PACKAGING AND TRANSMITTING RESULTS TO THE SAMPLE FILE CONTROL SYSTEM

The DMP system supports the generation of run results files for the EPA Sample File Control (SFC) data base management system. The analyst can initiate this process with the 'P' option at DMP command levels. The analyst is also responsible for identifying the reduced data files to be contained in the run results file and for transmitting the file to the appropriate device. Only reduced data files representing control standards (C), reagent blanks (R), and unknowns (U) can be transmitted to the SFC system. Spikes and duplicates are transmitted as unknowns.

9.1 GENERATING THE RUN RESULTS FILE

On entering the run results file packaging module (DMPR) the program immediately creates a run results file name in the form YYMMDDHHMMSS.RR. It then prompts for the user's initials and the seven character PARMETH code governing the run of samples being reported. An instrument/lab identifier is also requested. Both the PARMETH code and instrument identifier must coincide with a code and an identifier present in the SFC system.

The program next prompts the analyst for a name entry mode. Reduced data file names may be entered manually (M) or by namelist (L). In either case, the program will use the name or names to generate run results data. It will continue to prompt the analyst for names or namelists until the

analyst exits the session with the 'X' option. Figure 9.1 shows an example session. The program displays the header information of each file that it processes. After the file has been generated, the analyst is asked if quality control limits are to be appended to the file. This activity may be required by some laboratories to evaluate the precision and accuracy of the reported data.

9.2 SENDING RUN RESULTS TO THE SFC SYSTEM

Three ways have been devised for transmitting run results data to the SFC system. Only the tape transfer and the NOVA 840 option are currently available. An example tape transfer session is shown in Figure 9.2.a. Since it is possible to output more than one run results file to a tape, the user is given the opportunity to identify the tape file number on which the current run results file is to be written. During this operation, the user will be prompted to select whether he desires the run results file printed at the line printer and whether the file should be deleted once the file is written to tape. It is very important that each INCOS file name and its tape file number be recorded and affixed to the tape. Once all desired data has been transferred to tape, it may be shipped to the SFC computer and processed with a special tape utility.

The NOVA 840 option runs exactly like the tape option until the run results output selection is requested. An interface box designed at

EXAMPLE DMPL SESSION

DATE MANAGEMENT PROCESS COMMAND LEVEL (DMPC)

```
  DMP COMMAND (GERPQUXH):   [H]   > P

RUN RESULTS FILE GENERATION MODULE (DMPP1)
RUN RESULTS FILE NAME IS: 8211240935.RR
ENTER YOUR INITIALS  [INTS]  > DPR
ENTER GENERIC PARMETHO CODE  [XXXYZMN]   > 6250033
ENTER INSTRUMENT IDENTIFIER  [4096]   >
  PROCESS MODES:
    L - NAME LIST SAMPLE NAME ENTRY
    M - MANUAL SAMPLE NAME ENTRY
    X - EXIT TO SEND MODULE
    D - EXIT WITHOUT ACTION
  L, M, OR X   M   > L
NAME OF LIST FILE  [QDATA]   > MANY

RUN RESULTS NOW BEING GENERATED FOR SAMPLE: TEST00U
  SFC SAMPLE ID: 80-00111          SAMPLE TYPE: X
  UNITS: UG/L                      QC/MT NAME: 62501Q2
  SAMPLE VOLUME:       1.000 L     FACTOR:                1.000
  EXTRACTED: MM/DD/YY              INJECTED: 04/15/81
  EXTRACTION VOLUME:   1.000 ML    INJECTION VOLUME:      1.000 UL
  ANALYST: KERNS                   INSTRUMENT: FINN
  REAGENT BLANK: MIX10R            CONTROL STANDARD: MIX10C

NOW GENERATING RUN RESULTS FOR PRIMARY SAMPLE
NOW GENERATING RUN RESULTS FOR DUPLICATE
NOW GENERATING RUN RESULTS FOR SPIKE

RUN RESULTS NOW EING GENERATED FOR SAMPLE: TEST01U
  SFC SAMPLE ID: 80-00113          SAMPLE TYPE: U
  UNITS: UG/L                      QC/MT NAME: 62501Q2
  SAMPLE VOLUME:       1.000 L     FACTOR:                1.000
  EXTRACTED: MM/DD/YY              INJECTED: 04/15/81
  EXTRACTION VOLUME:   1.000 ML    INJECTION VOLUME:      1.000 UL
  ANALYST: DPR                     INSTRUMENT: FINN
  REAGENT BLANK: 0123456789        CONTROL STANDARD: 0123456789

NOW GENERATING RUN RESULTS FOR PRIMARY SAMPLE
PROCESS MODES:
    L - NAMELIST SAMPLE NAME ENTRY
    M - MANUAL SAMPLE NAME ENTRY
    X - EXIT TO SEND MODULE
    D - EXIT WITHOUT ACTION
  L, M, OR X  [M]  > L
```

Figure 9.1

```
PROCESS MODES:
    L - NAMELIST SAMPLE NAME ENTRY
    M - MANUAL SAMPLE NAME ENTRY
    X - EXIT TO SEND MODULE
    D - EXIT WITHOUT ACTION
  L, M, OR X [ M ] >  L

RUN RESULTS FILE HAS   255 RECORDS
WITH DATA FOR    4 SAMPLES.
THERE ARE    0 QUAL BLOCKS
AND    3 DISTINCT PARTYPES USED.
RRNAME:  8212081702.RR     DATE: 12/09/82
IQLNM:       3
PARMETH:  62501Q2.QC       U
PARMETH:  62501Q2.QC       D
PARMETH:  62501Q2.QC       F
PRDATE: 12/08/82    MATCHDT: 8212081704

RUN RESULTS APPEND AND SEND MODULE (DMPP2)
RUN RESULTS FILE NAME: 8212081702.RR
 APPEND QC LIMITS TO RR FILE [ N ] >
RUN RESULTS OUTPUT OPTIONS:
 T - COPY TO TAPE
 N - SEND TO NOVA VIA MICRO BUFFER
 P - SEND TO PDP 11/70 VIA MICRO BUFFER
 OPTION (T, N, OR P) [ T ]  >  T

MOUNT MAG TAPE AND INITIALIZE.
OUTPUT RR FILE TO MT:   [ 1 ]  > 1

 DISMOUNT TAPE AND RECORD RR FILES OUTPUT

 OUTPUT RUN RESULTS TO LINEPRINTER [ N ]  >
 DELETE RUN RESULTS FILE FROM DISK [ N ]  > Y
```

Figure 9.2a

EMSL-Cincinnati must be connected between the terminal being used and the NOVA computer of the INCOS system. This interface box also connects to a microcomputer which temporarily stores the run results data, then logs into the NOVA 840 computer and enters the data into the 840.

The microcomputer must be loaded with a compatible baud rate for the input port to be used and the five character start and stop codes recognized by the microcomputer. The start and stop codes must be compatible with the ones coded into the INCOS software. These codes are presently "START" and "/BOMB" for the respective start and stop codes.

The DMPP procedure prompts the user to turn on and off the interface at the appropriate times. The green light emitting diode (LED) indicates that the microcomputer is ready. The LED should be on before the carriage return is pressed for data transmission. If the green LED does not come on, the interface, lines and microcomputer should be checked before proceeding. As data is being transferred to the microcomputer, the "MICROCOMPUTER RECEIVING" LED should be lit and at the end of the transmission this LED should go off and the "MICROCOMPUTER STANDBY" LED should come on. At this point the run results data have been entered into the microcomputer and the operator can decide if he wishes it printed on the line printer and/or retained on the disk. An example microcomputer transfer session is shown in Figure 9.2b.

EXAMPLE SESSION NOVA 840 VIA
MICROCOMPUTER BUFFER TRANSFER

```
RUN RESULTS FILE HAS   255 RECORDS
WITH DATA FOR    4 SAMPLES.
THERE ARE    0 QUAL BLOCKS
AND    3 DISTINCT PARTYPES USED.
RRNAME:  8211240935.RR      DATE: 11/24/82
IQLNM:       3
PARMETH:  62501Q2.QC        U
PARMETH:  62501Q2.QC        D
PARMETH:  62501Q2.QC        F
PRDATE: 11/24/82    MATCHDT: 8211240938

RUN RESULTS APPEND AND SEND MODULE (DMPP2)
RUN RESULTS FILE NAME: 8211240935.RR
 APPEND QC LIMITS TO RR FILE [ N ] >
RUN RESULTS OUTPUT OPTIONS:
 T - COPY TO TAPE
 N - SEND TO NOVA VIA MICRO BUFFER
 P - SEND TO PDP 11/70 VIA MICRO BUFFER
 OPTION (T, N, OR P) [ T ]  >  N

SWITCH ON MICRO INTERFACE BOX
 PRESS RETURN WHEN READY [ CR ] >

TASK COMPLETE.  TURN OFF INTERFACE NOW

 OUTPUT RUN RESULTS TO LINEPRINTER [ N ]  >
 DELETE RUN RESULTS FILE FROM DISK [ N ]  >  Y
```

Figure 9.2b

SECTION 10

U - THE DMP UTILITY MODULE

The DMP utility module has not been implemented.